X1A: Second-generation undulator beamlines serving soft x-ray spectromicroscopy experiments at the NSLS


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The X1A undulator beamline is being rebuilt with two separate monochromators on its two branches. The new arrangement will deliver spatially coherent beams to imaging experiments, with spectral resolving power of up to 5000, and the capability to optimize the resolving power versus flux. The beamlines will operate simultaneously, and each will use 15 percent of the undulator beam, yet deliver high coherent flux. Because of the small beam divergence, the spherical grating monochromators can operate with fixed exit arms throughout the 250–800 eV range. © 1996 American Institute of Physics.

I. DESCRIPTION OF THE BEAMLINES

The X1A soft x-ray undulator, \( U \), gives high tunable flux from 200 to 800 eV. At a fixed gap setting, it provides considerable intensity over a broad spectral range, allowing several experiments to run simultaneously using different wavelengths. At the source, the beam has approximately Gaussian angular and spatial distributions in both the horizontal and the vertical planes, with \( \sigma_x = 430 \mu m \), \( \sigma_y = 7 \mu m \), \( \sigma_x' = 290 \mu rad \), and \( \sigma_y' = 24 \mu rad \).

The first mirror, \( M_0 \), is a scraper mirror that deflects around 35% of the beam towards our beamlines and leaves the rest to be used by the X1B beamline. This mirror is made of nickel-coated Glidcop and deflects the beam by 80 mrad.

The second set of mirrors, M1O and M1I, are toroidal optics that independently deflect and focus in the horizontal and vertical planes (O and I signify outboard and inboard branches). They each focus onto the monochromator entrance slits in the horizontal plane and onto the exit slits in the vertical plane. M1O is a scraper mirror that separates the inboard and outboard X1A beams. These mirrors are made of gold-coated silicon with horizontal and vertical radii of curvature \( r_{Ox} = 71.3 m \), \( r_{Oy} = 0.504 m \), \( r_{Ix} = 99.9 m \), and \( r_{Iy} = 0.424 m \), respectively. They are being fabricated by Continental Optical and will be positioned by McPherson manipulators, with provision for water cooling.

The entrance slits, ENSO and ENSI, act as sources for the monochromators. We can select one of several fixed slit widths, allowing a trade-off between resolution and flux by changing the source size for each monochromator. The entrance slit width options are 10, 25, 40, 70, 120, 200 \( \mu m \) and fully open for both beamlines. The slit assemblies will be water cooled.

The spherical gratings, GO and GI, disperse linearly with wavelength \( \lambda \) and refocus x-rays of the desired \( \lambda \) in the horizontal plane onto the exit slit. The gratings, being fabricated by Tayside Optical, have 900 lines per mm and a radius of 46 m. They deflect by 113.4 mrad and are made of gold-coated silicon. The depth of the laminar grooves, 11 nm, was chosen as the best compromise throughout our wavelength range. We can also mask the gratings in the horizontal and vertical planes.

The exit slits, EXSO and EXSI, have continuously adjustable widths to satisfy the spatial coherence condition for our zone plates as described in section II. Both horizontal and vertical foci will be located at the exit slits.

The gratings will be operated in positive (inside) first order, \( m = 1 \) (the exit arms are then longer than the entrance arms). The upper limit on resolving power is not as severe as it would be for \( m = -1 \) and a wider wavelength range can...
be used. This arrangement implies lower power density on the grating since the grating rotates toward more grazing angles.

We use zone plates as imaging optics for our microscopes. There will be both a developmental and a cryogenic scanning transmission x-ray microscope\(^8,9\) on the outboard branch (D-STXM and cryo-STXM). On the inboard branch, the scanning photoemission microscope\(^10\) (SPEM II) will be permanently installed, while portable diffraction\(^11\) and holography\(^12\) setups may also be placed there to intercept the beam.

The distances along the beamlines and angles of deflection for each optical element are given in Table I. A diagram summarizing the focusing functions of the elements for the outboard branch is shown in Fig. 1. A drawing of the beamline floor layout is shown in Fig. 2.

A new preparation lab will be located next to the experimental area, making sample preparation fast and convenient. The expansion of the floor space provides improved separation between the inboard and outboard branches and increased room for experiments.

Table I. Distances from the undulator along the beam and deflection angles.

<table>
<thead>
<tr>
<th>Element</th>
<th>Outboard Branch</th>
<th>Inboard Branch</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Distance (m)</td>
<td>Angle (mrad)</td>
</tr>
<tr>
<td>Mirror M0</td>
<td>12.95</td>
<td>80.0</td>
</tr>
<tr>
<td>Mirrors M1O,</td>
<td>16.30</td>
<td>100.0</td>
</tr>
<tr>
<td>M1I</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Entrance Slits</td>
<td>18.30</td>
<td>0.0</td>
</tr>
<tr>
<td>ENSO, ENSI</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gratings GO,</td>
<td>19.70</td>
<td>113.4</td>
</tr>
<tr>
<td>GI</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Exit Slits EXSO, EXSI</td>
<td>23.60</td>
<td>0.0</td>
</tr>
<tr>
<td>D-STXM</td>
<td>24.80</td>
<td>0.0</td>
</tr>
<tr>
<td>CryoSTXM</td>
<td>25.80</td>
<td>0.0</td>
</tr>
<tr>
<td>SPEM II</td>
<td>27.15</td>
<td>0.0</td>
</tr>
</tbody>
</table>

FIG. 1. The focusing diagram for the outboard branch in both the horizontal and vertical planes (not to scale). Labels are referred to in Table I.

II. SPATIAL COHERENCE CONDITION

We must satisfy certain spatial coherence requirements to assure a diffraction-limited spot size with our zone plates. The criterion we use for spatial coherence both vertically and horizontally is

\[
s' \theta \leq p \lambda ,
\]

where \(s'\) is the source size, \(\theta\) is the angular subtention of the zone plate, and \(p\) is a phase space parameter that ranges between 0.5 for high resolution contrast and 1.5 for low.\(^13\)

The effective source is at the exit slit. The angular subtention varies between the experiments because the zone plate diameters and distances to the exit slits vary. The vertical beam FWHM of the beam at the exit slit is also different for the two branches. Therefore estimates of coherence, monochromator resolving power and flux will vary between the experiments. For this paper we will only display these estimates for STXM.

The fractional number of modes incident on the zone plate vertically and horizontally for a given phase space parameter is

\[
n = \frac{s' \theta}{p \lambda} .
\]

When \(n \leq 1\) the spatial coherence condition is satisfied, but, when \(n < 1\), we waste flux. In practice, we will force \(n = 1\) in the horizontal by changing the exit slit width linearly with \(\lambda\) and have chosen the distance between exit slit and zone plate to keep \(n\) close to 1 in our wavelength range.

Since the horizontal focus of the grating stays near the exit slit as described in section III, an exit slit width of \(s' = 25\ \mu m\) works reasonably well for \(p = 0.5\). The angle \(\theta\) is fixed by the zone plate diameter (90 \(\mu m\) for D-STXM and CryoSTXM, 150 \(\mu m\) for SPEM II) and distance from the exit slit. The entrance slit and grating mask have no effect on the spatial coherence at the zone plate when the exit slit width is smaller than the image of the entrance slit and will control only the energy resolution versus flux trade-off. In this way, we make spatial coherence control independent of energy.
resolution and flux control. The fractional number of modes in the horizontal plane incident on the zone plate in STXM as a function of wavelength for \( p = 0.5 \) is shown in Fig. 3.

We want to overfill the zone plate with several coherent modes to make the instruments less sensitive to drift. The number of spatially coherent modes in the beam is again \( n \), where \( \theta \) is instead the angular divergence FWHM of the source.

The number of modes in the horizontal plane at the zone plate is found by starting at the undulator, then subtracting modes lost in the optics. The number of modes at the undulator in this plane, usually around 100, is determined mostly by the electron beam size and divergence. The first two mirrors and grating masks reduce the angular divergence, and the exit slit cuts part of the image. The entrance slit has no effect on the number of modes as long as its image is larger than the exit slit.

In the vertical plane, the image of the undulator will be at the exit slits. The image’s vertical FWHM at the exit slit is the source size for the zone plate. The number of modes in the vertical plane is due to the undulator alone. The zero emittance contribution to the total source size and divergence of the undulator beam is comparable to the electron beam contribution and must be considered. The fractional number of modes in the horizontal incident on the zone plate in STXM is also shown in Fig. 3.

III. MONOCHROMATOR RESOLVING POWER

There are several reasons why we need good energy resolving power. Quantitative mapping of chemical states using x-ray absorption near edge structure (XANES) requires a resolving power, \( \lambda / \Delta \lambda \), of up to 5000. Good resolution is also important for x-ray photoemission spectroscopy (XPS) with the photoemission microscope, SPEM. A resolving power on the order of the number of zones (around 500) minimizes chromatic aberration of the zone plate focus. To obtain a low wavelength spread \( \Delta \lambda_A \) due to aberrations, the defocus term \( F_{20} \) must be close to zero in our wavelength range. If we satisfy the Rowland condition only at, for example, \( \lambda = 33 \AA \), then \( F_{20} = 0 \) and \( \frac{\partial F_{20}}{\partial \lambda} = 0 \) only at that wavelength.

Because we desire a particularly good resolution at the carbon and oxygen K absorption edges for XANES purposes, we fix the exit arm length \( r' \) so that \( F_{20} = 0 \) at both 44 Å and 23 Å. Using this defocused Rowland condition, \( F_{20} \) stays closer to zero over most of our wavelength range than if we satisfied the Rowland condition for \( \lambda = 33 \AA \). This has the effect of keeping the horizontal focus close to the exit slit.

For both \( \Delta \lambda_A \) and the diffraction-limited wavelength spread, \( \Delta \lambda_D \), the width \( w = N \delta \) of the grating that the experiment, not the exit slit, sees is critical. The width depends on the degree of grating masking \( w_m = x / \cos \alpha \), where \( x \) is the horizontal masking width and \( \alpha \) is the incident angle. It can also depend on back-masking due to the angular acceptance of the zone plate and the diffraction width

\[
wd = \sqrt{\left(\frac{r'\theta}{\cos \beta}\right)^2 + \left(\frac{r'\lambda}{s' \cos \beta}\right)^2}
\]

where \( \beta \) is the diffracted angle. The actual width \( w \) is the smaller of \( w_m \) and \( w_d \). A reduction of \( w \) has a greater positive effect of reducing \( \Delta \lambda_A \) than a negative effect of increasing \( \Delta \lambda_D \) in our range, decreasing the energy bandwidth and increasing the resolving power.

Since the exit slit essentially determines spatial coherence, we trade off resolving power with flux at the entrance slit. Fig. 4 shows the monochromator resolving power on STXM as a function of energy for four fixed entrance slit sizes, the exit slit set at 25 \( \mu \)m and using \( w_d \).
IV. FLUX AT THE ZONE PLATE

A higher photon rate allows us to take faster images with the same signal-to-noise ratio, therefore we want to maximize the number of photons per second at the experiment. We fix the fraction of a mode incident on the zone plate with the exit slit. The photon rate is roughly linearly proportional to the bandwidth seen by the zone plate, which is a function of wavelength, entrance slit size $s$ and grating mask width $x$.

To calculate the flux at the zone plate, we assume optimum brightness for a given wavelength at the undulator. We then multiply this by the horizontal and vertical emittance and the bandwidth to find an intensity. We then multiply this intensity by the efficiency of the grating and the reflectivities of the mirrors. From this we get Fig. 5 for STXM and the same exit slit and entrance slit sizes as in Fig. 4.

V. CONCLUSION

The image at the exit slit and tolerances on the toroidal mirror angles were checked with SHADOW. The optical elements, their mounts and chambers are under construction. Each optical mount has been designed to minimize vibration that would affect the position, flux, and wavelength of the beam with respect to our experiments. We expect to begin rebuilding the X1A beamline in the spring of 1996. We look forward to running improved soft X-ray spectromicroscopy experiments when the second-generation beamlines at X1A are complete.

FIG. 5. Photon rate incident on the STXM zone plate with a 25 µm exit slit and entrance slit widths of 10, 25, 40, 70, 120 µm and fully open. The pair of peaks corresponds to using different harmonics of the undulator.

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